

Claims:

1. NMR-based method comprising generating a NMR spectrum of a mixture
5 comprising at least one hyperpolarised ligand, a target and optionally at least one further ligand or a hyperpolarised target and at least one ligand and comparing said NMR spectrum with a reference spectrum of the at least one hyperpolarised ligand or the hyperpolarised target.
- 10 2. NMR-based method according to claim 1 comprising
 - a) hyperpolarising at least one ligand or a target,
 - b) forming a mixture by contacting the at least one hyperpolarised ligand with a target or a target and at least one further ligand or the hyperpolarised target with at least one ligand,
 - 15 c) generating a NMR spectrum of the mixture, and
 - d) comparing said NMR spectrum with a reference spectrum of the at least one hyperpolarised ligand or the hyperpolarised target.
3. Method according to claims 1 and 2 wherein the ligand is selected from the
20 group consisting of proteins, glycoproteins, lipoproteins, polypeptides, glycopolypeptides, lipopolypeptides, peptides, carbohydrates, nucleic acids or a part, a fragment or a complex thereof and small organic molecules.
4. Method according to claims 1 to 3 wherein the ligands is a small organic
25 molecule of less than 2000 Da.
5. Method according to claims 1 to 4 wherein more than one hyperpolarised ligand is used.
- 30 6. Method according to claims 1 to 5 wherein the target is selected from the group consisting of proteins, glycoproteins, lipoproteins, nucleic acids, polypeptides, glycopolypeptides, lipopolypeptides, peptides or a part, a fragment or a complex thereof.

7. Method according to claims 1 to 6 wherein the at least one hyperpolarised ligand or the hyperpolarised target is an isotopically enriched ligand or target.
8. Method according to claims 1 to 7 wherein the at least one hyperpolarised
5 ligand or the hyperpolarised target is selectively isotopically enriched at one or more sites in the molecule.
9. Method according to claim 8 wherein the at least one hyperpolarised ligand or the hyperpolarised target is selectively isotopically enriched at one site in the
10 molecule with ^{13}C or ^{15}N .
10. Method according to claim 9 wherein the enrichment is a ^{13}C -enrichment.
11. Method according to claims 1 to 10 wherein the NMR spectrum generated is
15 a one-dimensional NMR spectrum
12. Method according to claims 1 to 11 wherein the NMR spectrum generated is generated using low flip angles.
- 20 13. Method according to claims 1 to 12 wherein the comparison with the reference spectrum shows a chemical shift difference, a relaxation time difference or a NOE effect difference.
14. Use of hyperpolarised ligands and/or hyperpolarised targets in NMR assisted
25 drug discovery.
15. Use of isotopically enriched hyperpolarised ligands in ligand competition assays.